

2-METHYLHEXANEDIOIC ACID  
33659-32-4 | DTXSID20334839

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.08e-07 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.64e-01

Confidence level: 5.88e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Piperazine</div> <div>Measured: 9.00e-08</div> <div>Predicted: 7.31e-01</div>	<div>Image not found</div> <div>Diallylamine</div> <div>Measured: 3.18e-07</div> <div>Predicted: 27.5</div>	<div>Image not found</div> <div>Cycloheptanone</div> <div>Measured: 2.88e-07</div> <div>Predicted: 1.00</div>
<div>Image not found</div> <div>3-Methylbutyl acetate</div> <div>Measured: 1.07e-08</div> <div>Predicted: 6.64</div>	<div>Image not found</div> <div>2-Ethoxyethyl acetate</div> <div>Measured: 5.55e-08</div> <div>Predicted: 1.46</div>	